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CONTRIBUTION TO THE BENCHMARK FOR TERNARY MIXTURES: DETERMINATION OF Soret COEFFICIENTS BY THE THERMOGRAVITATIONAL AND THE SLIDING SYMMETRIC TUBES TECHNIQUES.

Miren Larrañaga¹, M. Mounir Bou-Ali^{1a}, David Alonso de Mezquía¹, D. Andrew S. Rees², Jose Antonio Madariaga³, Carlos Santamaría³, Jean K. Platten⁴

¹MGEP Mondragon Goi Eskola Politeknikoa, Mechanical and Industrial Manufacturing Department, Loramendi 4 Apdo 23, 20500 Mondragon, Spain

²Department of Mechanical Engineering, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom

³Department of Applied Physics II, University of Basque Country, Apdo. 644, 48080 Bilbao, Spain

⁴University of Mons-Hainaut, B-7000 Mons, Belgium

^ambouali@mondragon.edu

Abstract

This work is part of an international project for the research on the transport properties in ternary mixtures. Six different teams have analysed the same mixture by independent techniques in order to compare the results and validate the techniques. This work is the contribution of the team of Mondragon Unibertsitatea for ground conditions measurements. This team has measured the thermodiffusion coefficients by the thermogravitational techniques and the molecular diffusion coefficients by the Sliding Symmetric Tubes technique. The Soret coefficients have been determined by the combination of the thermodiffusion and molecular diffusion coefficients. The mixture chosen for the study is the one formed by 1,2,3,4-tetrahydronaphthalene, isobutylbenzene and n-dodecane at mass fraction of 80% of THN, 10% of IBB and 10% of nC₁₂, and at 25°C. The good agreement between the results of the different teams shows the validity of the techniques used in this work.

1. Introduction

The research on transport properties in multicomponent mixtures is of great interest in the scientific community, due to their presence in lots of natural and industrial processes.

The case of binary mixtures has been widely studied, and there are several experimental techniques [1, 2] and numerical prediction models [3, 4] that allow the accurate determination the diffusion, thermodiffusion and Soret coefficients. Nowadays, the focus is on ternary mixtures, because it is necessary to analyse and understand them before going to multicomponent mixtures. In the last years, some works have been published which try to determine the thermodiffusion, molecular diffusion or Soret coefficients in ternary mixtures [5-14]. However, as they are individual works and not all concerned with the same mixture, there was a high dispersion between the results, so they were not easily comparable. Moreover, the existing differences in the theories about the thermodiffusion phenomenon in ternary mixtures [15-18] show again the need of a database of reliable experimental data. Because of these reasons, and in the framework of the project DCMIX (Diffusion coefficient measurements in ternary mixtures), this Benchmark in ternary mixtures has been developed, where six teams at international level have participated. The present work is published together with other five works corresponding to the other participant teams, and with another one more work in which a summary of the Benchmark is presented.

The purpose of this Benchmark is to analyse independently the same mixture by different techniques so that reliable results of thermodiffusion, molecular diffusion and Soret coefficients are provided. The chosen mixture is formed by 1,2,3,4-tetrahydronaphthalene (THN),

isobutylbenzene (IBB) and n-dodecane (nC₁₂) at mass fraction of 80% of THN, 10% of IBB and 10% of nC₁₂, and at 25°C. As was proposed in [2], the order of components chosen is in decreasing order of density, this is, THN-IBB-nC₁₂. The techniques which were employed to analyse this mixture are: Optical Beam Deflection technique (OBD) [6], which determines the Soret coefficients; the Taylor Dispersion instrument (TDT) [5] which determines the molecular diffusion coefficients, Optical Digital Interferometry (ODI) [5], which determines the Soret coefficients; the Open Ended Capillary (OEC) [7] which determines the molecular diffusion coefficients; the thermogravitational technique (TG) [8] which determines the thermodiffusion coefficients; and the Sliding Symmetric Tubes technique (SST) [9], which determines the molecular diffusion coefficients. In addition, measurements have been also performed in the SODI instrument (Selectable Optical Diagnostic Instrument) [18-19] on board the International Space Station (ISS); there, Soret coefficients can be determined in microgravity conditions. The Benchmark results in microgravity conditions have been analysed independently by four teams.

In the present work we present the contribution of the team at Mondragon Unibertsitatea and provide a detailed explanation of the processes used. More specifically, the thermodiffusion coefficients were determined by the thermogravitational technique, the molecular diffusion coefficients were determined by the Sliding Symmetric Tubes technique and Soret coefficients by the combination of the thermodiffusion and molecular diffusion coefficients.

2. Experimental procedure

In this section first, we describe the equipment used to measure the relevant thermophysical properties of the studied mixture composed by THN-IBB-nC₁₂ at mass fraction of 0.8-0.1-0.1. We describe also the procedure needed to determine the concentration of each component in a ternary mixture from the density and the refractive index. Then, the thermogravitational technique and Sliding Symmetric Tubes technique are described. Finally, the determination of the Soret coefficient is shown.

2.1. Thermophysical properties and experimental analysis

Before the determination of the thermodiffusion coefficient, it is necessary to determine also the density, the refractive index, the thermal expansion coefficient and the viscosity of the mixture. For the determination of the density an Anton Paar DMA 5000 vibrating quartz U-tube densimeter with accuracy of 5×10^{-6} g/cm³ was used. By measuring the density at different temperatures (24°C, 24.5°C, 25°C, 25.5°C, 26°C) the thermal expansion coefficient was deduced. Coupled to the densimeter is an Anton Paar RXA 156 refractometer with accuracy of 2×10^{-5} RIU, which measures the refractive index. By the measurements of density and refractive index we determine the concentration of the mixture. The dynamic viscosity was measured by an Anton Paar AMVn falling ball microviscometer, which has an accuracy of ± 0.002 seconds.

In order to determine the concentration of each component in a ternary mixture it is necessary to carry out a prior calibration. This calibration consists on preparing 25 mixtures with concentration around the concentration of study and measuring their densities and refractive indices. With this data, calibration planes are built (Fig.1 and Fig. 2) and from them, calibration parameters can be determined. These coefficients enable the determination of the concentrations of each component in a ternary mixture from the measurements of density and refractive index, by these equations:

$$c_1 = \frac{c'(\rho - a) - c(n_D - a')}{bc' - b'c} \quad (1)$$

$$c_2 = \frac{b(n_D - a') - b'(\rho - a)}{bc' - b'c} \quad (2)$$

$$c_3 = 1 - c_1 - c_2 \quad (3)$$

where c_1, c_2 and c_3 are the concentrations of components 1, 2 and 3, ρ is the density of the mixture, n_D is the refractive index of the mixture, and a, a', b, b', c and c' are the calibration parameters.

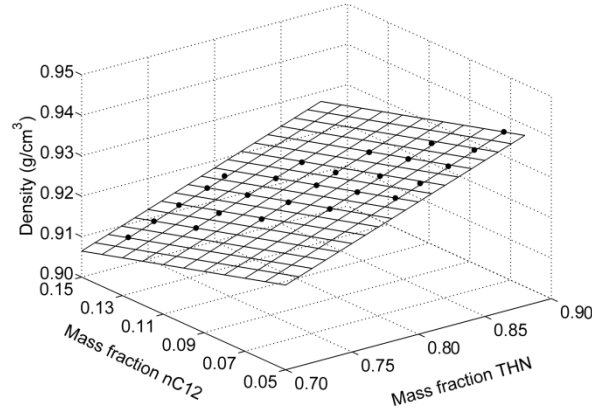


Fig. 1. Calibration plane of density for the mixture THN-IBB- nC_{12} at the mass fraction of 0.8-0.1-0.1 and at 25°C

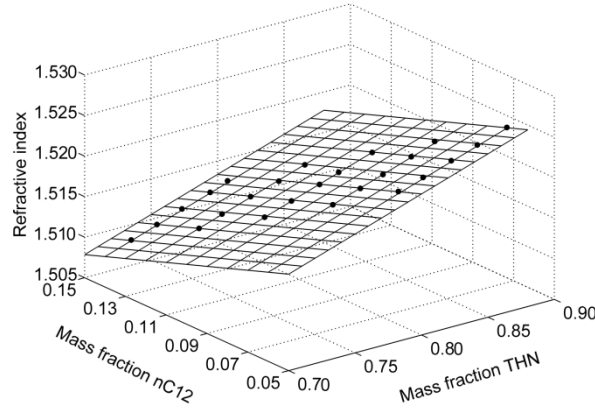


Fig. 2. Calibration plane of refractive index for the mixture THN-IBB- nC_{12} at the mass fraction of 0.8-0.1-0.1 and at 25°C

So as to validate the calibration, densities and refractive indices corresponding to each concentration are calculated by the calibration parameters. These calculated values are compared to the experimental ones. The maximum error admitted to validate a calibration is 0.5%.

2.2. Thermogravitational technique

The thermogravitational technique has been successfully used in several works, both in binary [20, 21] and ternary [8] mixtures. In this work two thermogravitational columns have been used: STC and LTC. Both of them have a very similar gap width, (STC has $L_x = 1 \pm 0.005$ mm and LTC has $L_x = 1.02 \pm 0.005$ mm) but different length. The first one has length of $L_z = 500$ mm (Fig. 3a), and it has been used in several works [8, 22, 23], whereas the second one has length of $L_z = 980$ mm (Fig. 3b) and therefore, produces a double separation. It has been designed and constructed with the aim of improving the accuracy in the determination of the concentration gradient, which is of particular interest for ternary mixtures.

This new column was validated by measuring the known Benchmark binary mixtures formed by THN, IBB and nC_{12} at 50% of mass fraction [8]. In all the cases, the differences with the

Benchmark values were under 3% (Table 1). Independently, in this work, the results obtained with both columns for the studied ternary mixtures are shown.

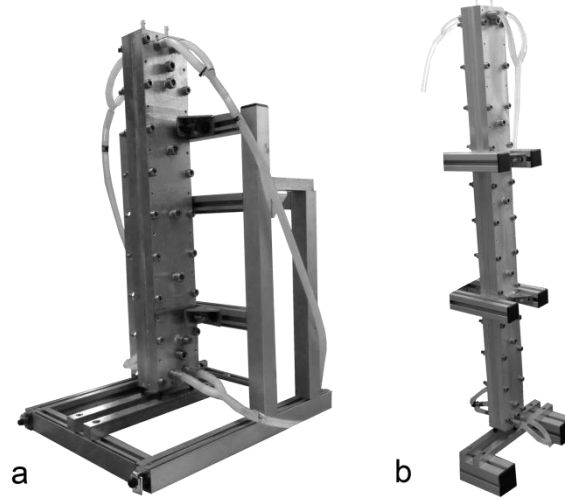


Fig. 3. a. Thermogravitational column of $L_z = 500$ mm (STC); b. Thermogravitational column of $L_z = 980$ mm (LTC)

Table 1. Comparison between Benchmark binary values and the experimental ones obtained by the thermogravitational column of $L_z = 980$ mm (LTC)

Mixture	$D_T \times 10^{-12}$ (m ² /sK) LTC	$D_T \times 10^{-12}$ (m ² /sK) Bench	Diff (%)
THN-IBB (0.5)	2.73±0.05	2.80	2.5
IBB- nC ₁₂ (0.5)	3.64±0.06	3.70	1.6
THN-nC ₁₂ (0.5)	6.05±0.10	5.90	2.5

In the thermogravitational technique, the analysed mixture is placed between two vertical walls at different temperatures. Due to the temperature gradient, generally, the denser component moves toward the colder wall, while the less dense component moves toward the hotter wall, thereby creating a concentration gradient. This gradient generates a diffusive flux in the opposite direction, due to the molecular diffusion effect. In addition, the effect of the gravity generates convective fluxes that amplify the separation along the column. When the ultimate stationary state is reached, density and refractive index are measured at different heights of the column (Fig. 4), which enables the determination of the variation of the concentration of each component along the height of the column (Fig. 5). These concentration gradients are used to determine the thermodiffusion coefficient for each component, by this equation [10]:

$$D'_{T,i} = - \frac{L_x^4}{504} \frac{\alpha g}{\nu} \frac{\partial c_i}{\partial z} \quad (4)$$

where $D'_{T,i}$ is the thermodiffusion coefficient for component i , L_x is the width of the gap of the column, ν is the kinematic viscosity of the mixture, α is the thermal expansion coefficient, g is gravity and $\partial c_i / \partial z$ is the variation of the concentration with the height of the column.

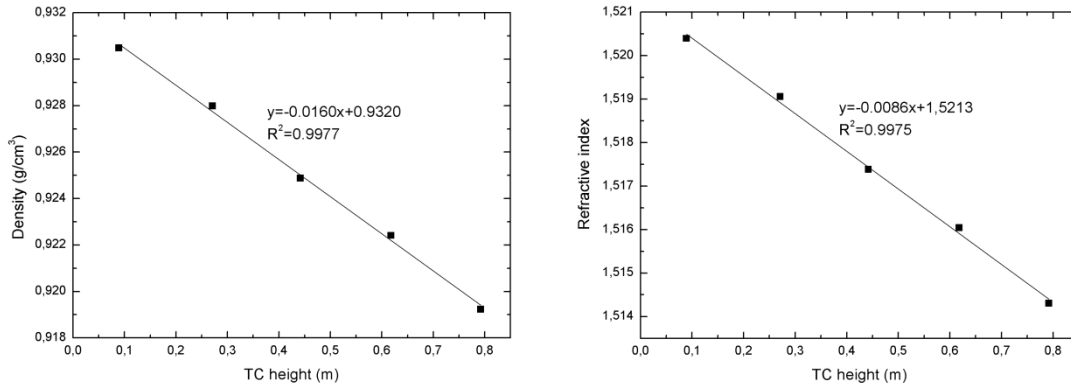


Fig. 4. Variation of the density and the refractive index of the mixture with the height of the column of $L_z = 980$ mm

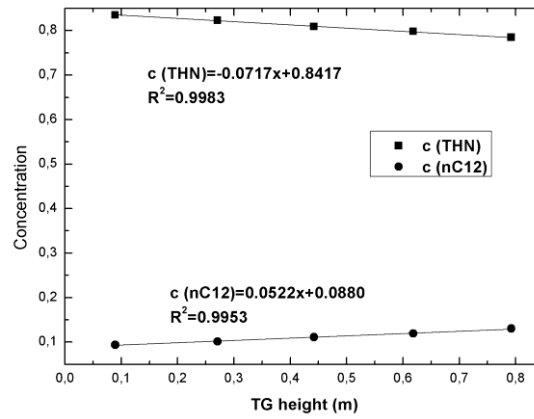


Fig. 5. Variation of the concentration of components 1 and 3 with the height of the column of $L_z = 980$ mm

The experimental error of each of the parameters in Eq.(4) must be considered when analysing the uncertainty of the determination of the thermodiffusion coefficients by the thermogravitational technique. As may be noticed, the geometric error of the width of the gap has the greatest influence, and it will appear in all the measurements made by the column. In the case of the thermal expansion coefficient, the accuracy of the densimeter and the error of the linear regression (density vs temperature) were considered. The errors of the density and the dynamic viscosity are directly related to the accuracy of the densimeter and the microviscometer respectively. Finally, in the case of the concentration gradients, two facts were considered: the calibration errors and the accuracy of the linear regressions (concentration vs height).

2.3. Sliding Symmetric Tubes technique

This technique has been employed in several works in order to determine the molecular diffusion coefficients in both binary [24] and ternary mixtures [9], where the procedure for determining the molecular diffusion coefficients is widely described. In Fig. 6 the installation used for the SST technique is shown.



Fig. 6. Installation for the Sliding Symmetric Tubes technique

By this technique, molecular diffusion coefficients can be determined from the variation of the concentration of each component with time. The slopes of the linear regressions formed when showing the variation of the concentration with the square root of time, enable the determination of the molecular diffusion coefficients by the following working equations:

$$S_1 = \frac{2}{L\sqrt{\pi}} \left(\frac{A}{\alpha_1} + \frac{B}{\alpha_2} \right) \quad (6)$$

$$S_2 = \frac{2}{L\sqrt{\pi}} \left(\frac{A}{\alpha_1} \left(\frac{1-D_{11}\alpha_1^2}{D_{12}\alpha_1^2} \right) + \frac{B}{\alpha_2} \left(\frac{1-D_{11}\alpha_2^2}{D_{12}\alpha_2^2} \right) \right) \quad (7)$$

where S_1 and S_2 are the slopes formed by the variation of the concentration with the square root of time, L is the length of the tubes, A and B are the integration constants, α_1 and α_2 are function of the eigenvalues of the diffusion matrix, D_{11} and D_{22} are the diagonal diffusion coefficients and D_{12} and D_{21} are the cross-diagonal diffusion coefficients.

As it is detailed in [9], two independent experiments with different initial concentrations are needed to determine the molecular diffusion coefficients of a ternary mixture. Thus, we have four equations and four unknowns: the four molecular diffusion coefficients. In order to solve the system, the Newton-Raphson method is used, where the fitting parameters are the four diffusion coefficients. We can control the maximum fitting error in order to be under 1%.

To determine the experimental error in the determination of the molecular diffusion coefficients by the SST technique, three factors may be taken into account: (i) the admitted error in the Newton-Raphson fitting, (ii) the fitting error of the linear regressions (concentration vs. square root of time) and (iii) the calibration error.

2.4. Determination of Soret coefficient

The Soret coefficient for each component, $S'_{T,1}$, $S'_{T,2}$, is determined from the results obtained for the molecular diffusion and thermodiffusion coefficients, by means of the following equations [25]:

$$S'_{T,1} = \frac{D'_{T,1}D_{22}-D'_{T,2}D_{12}}{D_{11}D_{22}-D_{12}D_{21}}, \quad S'_{T,2} = \frac{D'_{T,2}D_{11}-D'_{T,1}D_{21}}{D_{11}D_{22}-D_{12}D_{21}} \quad (8)$$

The experimental error accumulated in the indirect determination of the Soret coefficient is obtained by applying the rules of error propagation in Eq. (8).

3. Results

In this section the results obtained for thermodiffusion, molecular diffusion and Soret coefficients for the mixture THN-IBB-nC₁₂ at mass fraction of 0.8-0.1-0.1 and at 25°C are shown. In addition, the results corresponding to the density, dynamic viscosity, thermal

expansion coefficient and calibration parameters used for the determination of the concentrations of each component of the mixture are presented at the beginning.

3.1. Thermophysical properties and calibration parameters

Table 2 gives the density, dynamic viscosity and thermal expansion coefficient of the chosen ternary mixture at the reference concentration.

Table 2. Density, thermal expansion coefficient and dynamic viscosity for the ternary mixture THN-IBB-nC₁₂ at mass fraction of 0.8-0.1-0.1 and at 25°C.

THN-IBB-nC ₁₂ <i>c₁-c₂-c₃</i>	ρ (kg/m ³)	$\alpha \times 10^{-3}$ (K ⁻¹)	μ (mPa·s)
0.8-0.1-0.1	925.316	0.848	1.719

Then, in Table 3 the calibration parameters necessary for the determination of the concentration gradient of each component in the mixture by Eq (1) and Eq (2) are shown.

Table 3. Calibration parameters for the ternary mixture THN-IBB-nC₁₂ at mass fraction of 0.8-0.1-0.1 and at 25°C.

THN-IBB-nC ₁₂ <i>c₁-c₂-c₃</i>	<i>a</i> (kg/m ³)	<i>b</i> (kg/m ³)	<i>c</i> (kg/m ³)	<i>a'</i>	<i>b'</i>	<i>c'</i>
0.8-0.1-0.1	845.888	117.569	-145.028	1.48294	0.05497	-0.09042

3.2. Thermodiffusion coefficients

As has been commented previously, in this work the thermodiffusion coefficients have been determined by two different thermogravitational columns: one with length of $L_z = 500$ mm and the other with length of $L_z = 980$ mm. Three independent experiments were performed in each column, from which the mean value is taken as the proposed result for the Benchmark. Table 4 shows the results for the components 1 and 3 (i.e. THN and nC₁₂). The standard deviation between the six experiments is of 1.4% for component 1 and of 3.6% for component 3 and as can be observed in Table 4, these deviations are within the experimental error bar. To determine the uncertainty of the proposed values, the experimental error has been taken into account.

The values of the thermodiffusion coefficient of IBB can be calculated from the condition that the sum of the three thermodiffusion coefficients is zero. In this mixture, this coefficient is positive and smaller than the other two.

Table 4. Thermodiffusion coefficients for the ternary mixture THN-IBB-nC₁₂ at mass fraction of 0.8-0.1-0.1 and at 25°C.

	$D'_{T,1} \times 10^{-12}$ (m ² /sK)	$D'_{T,3} \times 10^{-12}$ (m ² /sK)
STC $L_z = 500$ mm	0.68±0.03	-0.49±0.01
	0.66±0.05	-0.45±0.07
	0.66±0.03	-0.46±0.03
LTC $L_z = 980$ mm	0.67±0.04	-0.50±0.03
	0.69±0.03	-0.50±0.03
	0.68±0.04	-0.51±0.03
Proposed values	0.67±0.05	-0.49±0.06

3.3. Molecular diffusion coefficients and eigenvalues of the diffusion matrix

As was commented in the Section 2.3, it is necessary to perform two experiments with different initial concentrations in order to determine the molecular diffusion coefficients of one mixture. In this case, in order to check the repeatability of the SST technique, four independent

experiments were performed with different initial concentrations. Combining the data of the experiments, four cases of results can be obtained. In the following Table 5 the initial concentrations of the four experiments are shown.

Table 5. Initial concentrations of the experiments carried out by the SST technique

	Bottom tube			Upper tube		
	THN	IBB	nC ₁₂	THN	IBB	nC ₁₂
Exp. 1	0.84	0.08	0.08	0.76	0.12	0.12
Exp. 2	0.84	0.10	0.06	0.76	0.10	0.14
Exp. 3	0.85	0.07	0.08	0.75	0.13	0.12
Exp. 4	0.85	0.10	0.05	0.75	0.10	0.15

As can be observed, in the experiments 1 and 3 the concentrations of all the components vary, whereas in the experiments 2 and 4, the concentration of the IBB stays constant between the upper and the bottom tubes. In Fig. 7 the variation of the concentration of each component with the square root of the time is shown for two independent experiments.

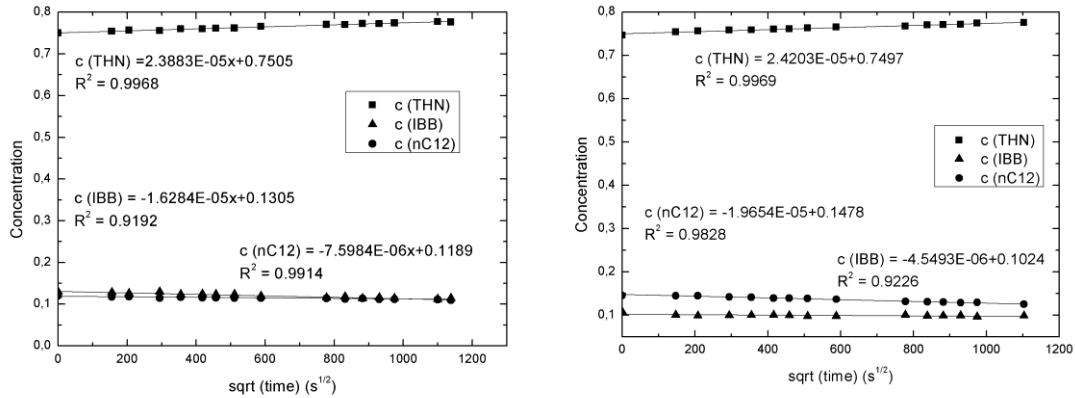


Fig. 7. Variation of the concentration of each component with the square root of the time, for the experiments 3 and 4, for the mixture THN-IBB-nC₁₂ at mass fraction of 0.8-0.1-0.1 and at 25°C.

Table 6 gives the results corresponding to the molecular diffusion coefficients and the eigenvalues of the diffusion matrix for the four possible combinations of experiments. In each case, the corresponding experimental error is given. The results shown are for the order of components THN-IBB-nC₁₂. The second digit after the decimal point is not relevant in most of the cases, but it has been kept in the results so as to maintain the consistency in this work and in the summary work.

Table 6. Molecular diffusion coefficients and eigenvalues of the diffusion matrix for the ternary mixture THN-IBB-nC₁₂ at mass fraction of 0.8-0.1-0.1 and at 25°C.

Experiments	$D_{11} \times 10^{-10}$ (m ² /s)	$D_{12} \times 10^{-10}$ (m ² /s)	$D_{21} \times 10^{-10}$ (m ² /s)	$D_{22} \times 10^{-10}$ (m ² /s)	$\widehat{D}_1 \times 10^{-10}$ (m ² /s)	$\widehat{D}_2 \times 10^{-10}$ (m ² /s)
1-2	4.91±0.62	-1.97±0.25	0.99±0.12	8.57±1.08	5.56±0.70	7.92±0.99
3-4	5.47±0.69	-1.87±0.23	-0.06±0.01	8.43±1.06	5.43±0.68	8.47±1.06
1-4	5.66±0.71	-0.42±0.53	-0.44±0.05	5.63±0.71	5.22±0.66	6.08±0.76
2-3	4.87±0.61	-2.95±0.37	1.08±0.14	10.49±1.32	5.50±0.67	9.85±0.12
Mean value	5.23±0.66	-1.80±0.23	0.39±0.05	8.28±1.00	5.43±0.68	8.08±1.02

As can be observed, in the case of the eigenvalues the repeatability is convincing, especially for \widehat{D}_1 . Regarding to the molecular diffusion coefficients, the D_{11} coefficients have an acceptable repeatability, but in the case of the other coefficients the repeatability is worse, finding even changes in the sign in the case of the D_{21} coefficient. Although it may not be wise to calculate

the mean values of the diffusion coefficients with such large deviations, we have done it and taken it as a fifth case of results. The purpose of this is to analyse the reliability of the Soret coefficients calculated by Eq. (8). The uncertainty given for these mean values is the experimental error.

3.4. Soret coefficients

Soret coefficients have been determined by Eq (8). In the previous section, a bad repeatability of the molecular diffusion coefficients has been observed. Therefore, Soret coefficients have been determined for the four possible results of molecular diffusion coefficients and also for their mean value. In the case of the thermodiffusion coefficient, the mean value of the results obtained by both columns has been used. The results are shown in Table 7.

Table 7. Soret coefficients for each case of molecular diffusion coefficients for the ternary mixture THN-IBB-nC₁₂ at mass fraction of 0.8-0.1-0.1 and at 25°C.

D'_{Ti}	D_{ij}	$S'_{T,i} \times 10^{-3} (K^{-1})$	$S'_{T,3} \times 10^{-3} (K^{-1})$
Mean value	Exp 1-2	1.23±0.09	-0.87±0.14
	Exp 3-4	1.16±0.09	-0.95±0.16
	Exp 1-4	1.17±0.09	-0.93±0.15
	Exp 2-3	1.20±0.09	-0.90±0.15
	Mean value of Dij	1.19±0.09	-0.91±0.15
	Proposed values	1.19±0.09	-0.91±0.15

As may be observed, although the molecular diffusion coefficients are quite different, in the case of Soret coefficients essentially the same results are obtained in the five cases. The standard deviation between the five cases is of 2.5% for component 1 and of 4.4% for component 3, and as can be observed in Table 7 the deviations are within the experimental error bars. This implies that the molecular diffusion coefficients, especially the cross-diagonal ones, have only a small influence on the Soret coefficients. The values proposed for Soret coefficients are the mean values of the five cases analysed, with the corresponding experimental error.

4. Conclusions

The thermophysical properties, the eigenvalues of the diffusion matrix and the thermodiffusion, molecular diffusion and Soret coefficients have been determined for the ternary mixture THN-IBB-nC₁₂ at mass fraction of 0.8-0.1-0.1 and at 25°C. Table 8 shows the values for the thermodiffusion, molecular diffusion and Soret coefficients and for the eigenvalues of the diffusion matrix proposed by the team of Mondragon Unibertsitatea for the Benchmark

Table 8. Proposed values by the team of Mondragon Unibertsitatea for thermodiffusion, molecular diffusion and Soret coefficients and for the eigenvalues of the diffusion matrix, for the ternary mixture THN-IBB-nC₁₂ at mass fraction of 0.8-0.1-0.1 and at 25°C.

$D'_{T,1} \times 10^{-12} (m^2/sK)$	$D'_{T,3} \times 10^{-12} (m^2/sK)$	$S'_{T,1} \times 10^{-3} (K^{-1})$	$S'_{T,3} \times 10^{-3} (K^{-1})$		
0.67±0.05	-0.49±0.06	1.19±0.09	-0.91±0.15		
$D_{11} \times 10^{-10} (m^2/s)$	$D_{12} \times 10^{-10} (m^2/s)$	$D_{21} \times 10^{-10} (m^2/s)$	$D_{22} \times 10^{-10} (m^2/s)$	$\widehat{D}_1 \times 10^{-10} (m^2/s)$	$\widehat{D}_2 \times 10^{-10} (m^2/s)$
5.23±0.66	-1.80±0.23	0.39±0.05	8.28±1.00	5.43±0.68	8.08±1.02

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